

# First Steps with UNIX in Life Sciences

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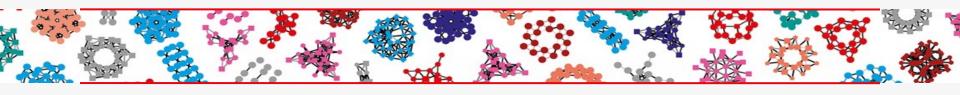




## Learning outcomes

- To get familiar with the UNIX environment
- To use the most common UNIX commands
- To acquire skills necessary for further courses requiring UNIX, like HPC and NGS analysis courses.

## **Outline**



- 1. What is UNIX and why should biologists use it?
- 2. UNIX filesystem: navigation and usage
- 3. Environment, processes & Jobs
- 4. Working with directories and files
- 5. Working with file content

Exercises are integrated in chapters

An optional exam will be put online at the end of the course

# What is UNIX and why should biologists use it?







# Command Line Interface (CLI)

In the 70's, all systems used a command line interface

```
Starting MS-DOS...
C:\>_
```



```
APPLE II

DOS VERSION 3.3 SYSTEM MASTER

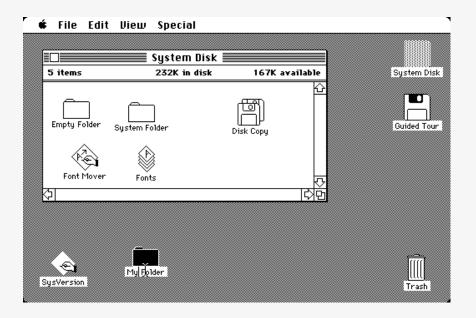
JANUARY 1, 1983

COPYRIGHT APPLE COMPUTER, INC. :980,1982

BESURE WARS COOK STOOMS
```

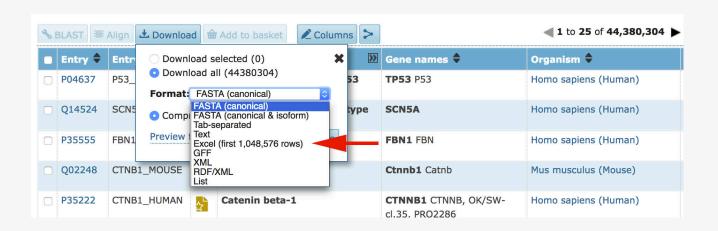
# Graphical User Interface (GUI)

- Development since the 60's
- First popular product was the Macintosh in 1984
- **Different way of thinking** / acting: windows, menus, icons, mouse and clicks (now touchscreens)

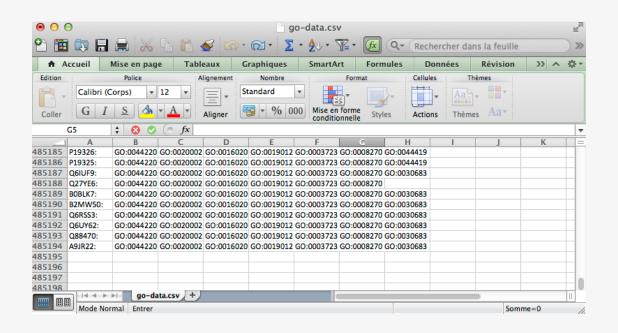


## CLI vs GUI – size issues

### Dealing with more than 1 million lines



# CLI vs GUI - complex queries



- How many Swiss-Prot Identifiers are in the file ?
- How many different GO annotations are there?
- What are the 4 most common GO annotations?

# CLI vs GUI - complex queries

How many Swiss-Prot identifiers?

```
userA$ wc -1 go-data.csv
485194
```

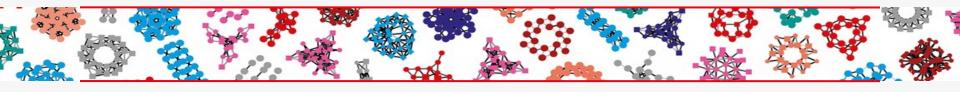
How many different GO annotations?

```
userA$ tr " " "\n" < go-data.csv | grep ^GO: | sort | uniq | wc -1 15696
```

What are the 4 most common GO annotations?

```
userA$ tr " " "\n" < go-data.csv | grep ^GO: | sort | uniq -c |
sort -nr | head -4
127303 GO:0005737
82740 GO:0005524
66591 GO:0016021
52952 GO:0046872</pre>
```

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# UNIX filesystem: navigation and usage



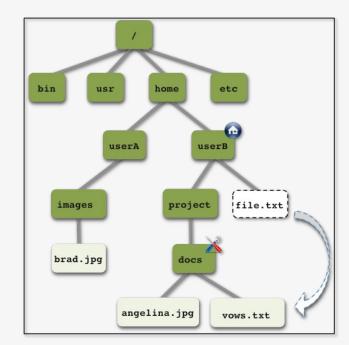


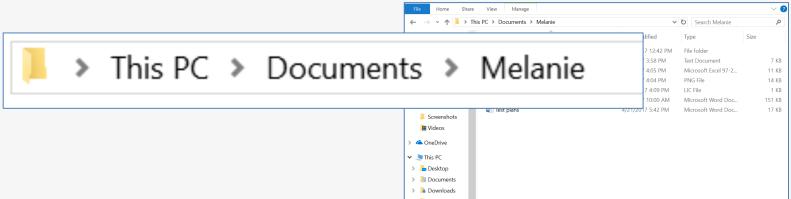


## Files & directories

- Organised as an inverted tree
- Single root '/' at the top.
- Directory: is a file containing file & directory names
- Home directory: is the 'private' directory of a user
- Working directory: is the current directory.

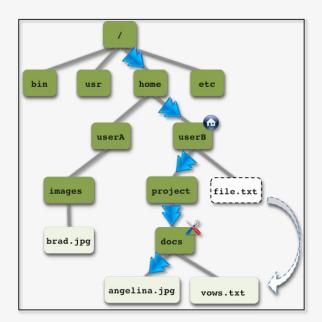
  The one you are in when executing a command.
- File: is a file





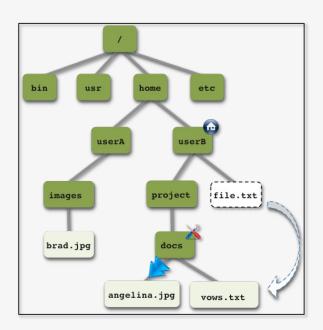
## **Paths**

### absolute path...



from the root

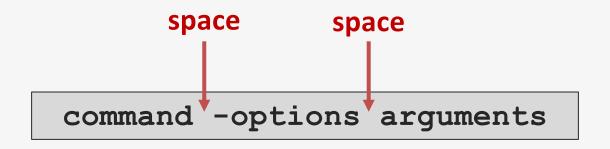
### relative path...



from the working directory

angelina.jpg

## General command syntax



By default, commands are executed in the working directory

## Help about commands & options

#### man

```
PWD(1)
                          BSD General Commands Manual
                                                                        PWD(1)
NAME
    pwd -- return working directory name
SYNOPSIS
     pwd [-L | -P]
DESCRIPTION
    The pwd utility writes the absolute pathname of the current working directory to the stan-
    dard output.
    Some shells may provide a builtin pwd command which is similar or identical to this util-
     ity. Consult the builtin(1) manual page.
    The options are as follows:
     -L
             Display the logical current working directory.
             Display the physical current working directory (all symbolic links resolved).
    If no options are specified, the -L option is assumed.
ENVIRONMENT
     Environment variables used by pwd:
     PWD Logical current working directory.
EXIT STATUS
    The pwd utility exits 0 on success, and >0 if an error occurs.
SEE ALSO
     builtin(1), cd(1), csh(1), sh(1), getcwd(3)
```

# Navigation - Locate

### pwd

- for 'print working directory'
- indicates the absolute path of the current directory

```
bin
          usr
                    home
                                etc
                            userB
            userA
                       project
                                  file.txt
   images
  brad.jpg
                        docs
              angelina.jpg
                                vows.txt
```

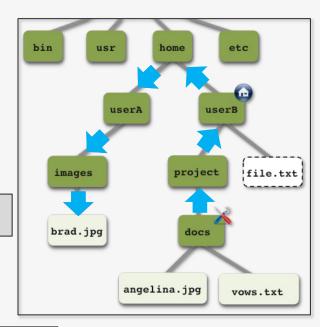
```
userB$ pwd
/home/userB/project/docs
```

# Current & parent directories

Example: the current directory is 'docs'

Absolute path to brad.jpg

/home/userA/images/brad.jpg



Relative path to brad.jpg

Parent directory

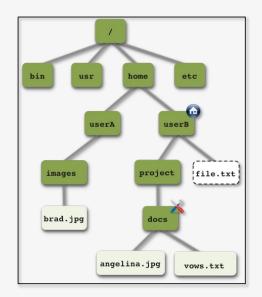
Copy brad.jpg to current directory

../../home/userA/images/brad.jpg

# **Navigation**

### cd

- for 'change directory'
- allows to navigate through the directories

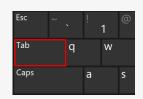


- o To go to the root: cd /
- To go to user home directory: cd ~ or just cd
- o To go up: cd ...
- o To go down: cd project/docs

# Navigation – Auto-completion

Current working directory: home

$$[command] + 1x$$



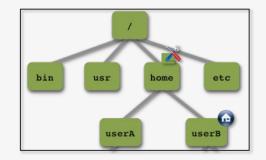


- Example: userA
  - userB





-> lists the content of the current directory



# Navigation – Auto-completion

Fast navigation

Safe commands

# Navigation – Content listing

### Is

- for 'list'
- displays the directories and files of the current directory or of a specified directory

#### **Options**

- -I shows one item per line, with detailed information, such as dates and access rights
- -h prints file and directory sizes in human readable format (combined with -l)
- -a shows all files, including hidden files
- -t sorts by modification time (most recent first), default sorting being by name
- -r reverts sorting
- -R shows content recursively

## Rules – case sensitivity

The command line differenciates upper from lower case letters:

brad.jpg

**≠** 

**BRAD**.jpg

**≠** 

brad.JPG

## Rules – filename limitations

Nearly no limitation in length or characters. However...

- forbidden character: /
- not recommended characters:
  - characters with a particular meaning for the shell: space ,;: \* ? & % \$ | ^ ~
     ' " () [] {}! \ #
  - international characters: é à æ ñ ç
- safe characters: \_ . 0-9 a-z

## Rules – filename extensions

File extensions are **arbitrary** and **do not have a particular meaning** for the operating system, but are useful for the users.

```
    .sh shell scripts
    .pl perl scripts
    .py python scripts
    .txt text files with no particular format
    .csv text files with Comma-Separated Values
    .fas files containing sequences in FASTA format*
```

\*FASTA is a text-based format for representing either nucleotide or peptide sequences.

## Rules – filename extensions

A file can have several extensions...

archive.tar.gz

archive.od.cw

...or no extension

tar = archive gz = compression



od = no meaning cw = no meaning

archive

## Users and permissions

Every file / directory has access properties

### who can access? 3 levels of classes:

**user** the file owner

group other users in the same group as the file owner

others all other users in the system

all users in the system

## Users and permissions

Every file / directory has access properties

### what kind of access? 3 access modes:

read permission to view the content of the file

write permission to edit the content of the file

**execute** permission to run a file (scripts, programs) or to

enter a directory

## Users and permissions

Every file / directory has access properties

### what restriction/permission?

- + adds the permission
- removes the permission
- applies the specified mode to the specified classes (faster if heterogeneous initial modes)

Root or system administrator has all rights!!!

### chmod

```
chmod [u g o a] [+ - =] [r w x] file_name

____user
____group
____write
execute
```

### **Option:**

-R recursive action

chmod can be run by root or by file owner only

```
-rwxrwxrwx file01.txt
-rwxrwxrwx file02.txt
```

How to allow everyone to read these files, but prevent 'group' + 'others' to 'write' and 'execute' them?

```
chmod go-wx file01.txt file02.txt
```

```
-rwxr--r-- file01.txt
-rwxr--r-- file02.txt
```

```
-rwxrwx--- file01.txt
-rwxr-xr-x file02.txt
```

How to allow everyone to read these files, but prevent 'group' + 'others' to 'write' and 'execute' them?

When several files with different permissions, it will be useful to set exact permissions using '='

```
chmod u=rwx,go=r-- file01.txt file02.txt
```

```
-rwxr--r-- file01.txt
-rwxr--r-- file02.txt
```

Each configuration of permission can be replaced by a code.

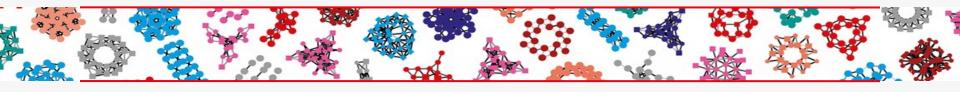
For example *chmod 700* = all permissions for owner, but none for all others ugo

Number	Octal Permission Representation	Ref
0	No permission	
1	Execute permission	X
2	Write permission	-W-
3	Execute and write permission: 1 (execute) + 2 (write) = 3	-wx
4	Read permission	r
5	Read and execute permission: 4 (read) + 1 (execute) = 5	r-x
6	Read and write permission: 4 (read) + 2 (write) = 6	rw-
7	All permissions: 4 (read) + 2 (write) + 1 (execute) = 7	rwx

### In a nutshell

- Files and directories are organised as a tree
  - Navigate along its branches with cd
  - List folders content with Is
- Commands are executed at the current working directory if a path is not specified
- Rules
  - Case sensitivity
  - Filename extensions are arbitrary
  - Characters with a meaning for the shell are not recommended
- Access permissions for reading, writing and execution

## **Outline**



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Exercises are integrated in chapters

# Environment, processes & Jobs







### User environment

#### man

Equivalent to help, often used to search commands' options

#### uname

Prints information about the system (several options)

### whoami, id, groups, who

Prints information of the user

# User environment

#### clear

This command allows to clean the screen

### history

Allows to view the history of previous commands, which are listed with an increasing number

Call the last command with: !!

Search a string with ctrl + r

Browse history with up and down arrows

View page by page history with history | less

Browse through the last commands with the UP and DOWN keys

## Alias

Regularly used complex commands can be renamed for simplification

#### Example:

alias la="ls -altr"

(list the content, including hidden files, ordered by reverse date)

- active only during the current session
- write it in a special file to make it permanent

### Job status

- Run in the foreground
  - prompt not available until the job ends
  - the output is displayed on the terminal
- Run in the background
  - add & after the command
  - the prompt remains available
  - the output is not displayed on the terminal
- Done
- Stopped
- Terminated / killed -> (CTRL -c, kill)
  - when a process does not behave as expected frozen, gone into a loop...
  - Use CTRL -c when in foreground to kill the current process
  - Use kill %[jobID] to kill a job in background

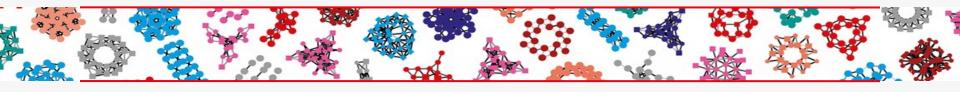




### In a nutshell

- Commands to get information about you and your environment
- History of the last previous commands
- Simplfy commands with alias
- Jobs can be running in foreground or background
- Kill a process / job with CTRL -c when you get stuck

# Outline



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# Working with directories and files







### Wildcard characters

are very useful for multiple files manipulation

```
*
     matches any number of characters in a file or directory name
     ls image*.jpeg ls *.jp*g
     matches exactly one character - use '??' to match any group of 2 characters
     1s *.???
     specify a range of characters allowed at that position – separated by an
     hyphen; use '!' to exclude a range of characters at that position
     ls [a-f]* ls [!a-f]*
     specify a list of terms - separated by commas
     ls *{.html,.txt}
```

#### mkdir

• "make directory": **creates** a new directory in the current directory mkdir new-directory(ies)

#### **Option**

-to create:

- several levels at a time: option –p
- several directories at a time with a path:
   mkdir level1/{level2a,level2b,level2c}
- several level with several directories
   mkdir -p 11/{L2a,L2b,L2c}

moves a file or a directory to a new location
 mv file-or-directory-name new-location/

renames a file or a directory
 mv file-or-directory-name new-name

Important: Moving files can overwrite existing files. -i option ask before overwritting



mv file1 file2

If no file2, file1 is renamed

If file2 exists, it's overwritten -> use option -i for confirm.



mv file1 directory2/ file1 is moved to directory2

mv file1 directory2 file1 is renamed directory2

Good Practice: autocompletion is useful to check if the new name or the new location exist

#### cp

- to make a <u>copy</u> of a file with another name cp file-name.txt file-name2.txt
- to make a copy of a file in another directory (same name is kept)
   cp file-name.txt Other\_directory/
- to copy a directory and all its files
   cp -R directory/ new-directory/

Important: Copying files can overwrite existing files. Use option -i

#### rm

• to remove/delete a file rm file-name.txt

#### rmdir

• to remove/delete a directory rmdir empty-directory-name/

Important: by default a directory must be empty before it can be deleted.

#### rm options

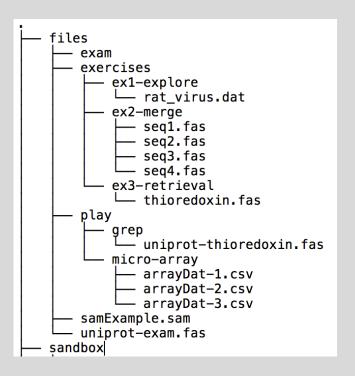
- -R or -r (for 'recursive')
   removes directories and their contents recursively
   rm -R non-empty-directory-name/
- -f (for '-force')
   never prompts for user confirmation, when files are writeprotected

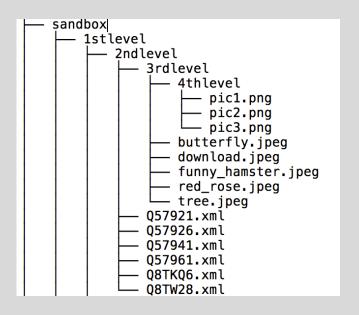
#### Use these options with care as there is no way back!

Hint: before executing a *rm* command with file names containing wildcard characters, simulate it first with the *ls* command as a control.

# File organization

#### tree





### Find files or directories

#### find

 Very effective in finding files & directories find [path] [query type] 'query term'

#### Path

- '.' to search in the current directory and its sub-directories
- '/' (root directory) to search in all directories
- Use single or multiple '.../' to search in parent directories
- '~' to search in your home directory

### Find files or directories

#### **Query types**

- -name for a search based on the file name
  - **-iname** same but case insensitive

```
find . -name '*.java'
```

- -type f or -type d to limit the search to files only or directories only
- -size [+,-]n[scale], for a search based on the file size, where...
   + stands for 'larger than', for 'smaller than', nothing for 'exact size',
   n indicates the numeric value,
   scale indicates the size: c for bytes; k for kilobytes; M for megabytes and G for gigabytes

```
find \cdot -size +50M
```

• -perm [permission code]

```
find . -perm 644
```

### Find files or directories

#### **Tips**

- Better to quote the query term with simple quotes
- Wildcards are possible
- ! placed after the path is the negative ("that do no match the criteria")
- Options can be combined
- Boolean operators (AND, OR) can be used in combination with find

```
find . -name '*.mpeg' -and -size +30M (default)
find . -name '*.png' -or -name '*.jpg'
find . \( -name '*.png' -or -name '*.jpg' \)
-and -size +30M
```

When multiple arguments, possible to use regular expressions (-regex option)

# File type determination

Reminder: file extensions do not have a particular meaning for the OS, thus might not correspond to the real file format

#### file

To check the **format** and detailed information of a file: *file filename(s)* 

- text the file contains only printing characters and a few common control characters
- executable the file contains the result of compiling a program
- data anything else (data is usually binary or non-printable)

### New file

#### touch

 creates a **new** empty file touch filename(s)

If *filename* already exists, this command does not erase file content, but updates its latest modification time

# Archiving and extracting data

#### tar

Creates, updates or expands archives

#### **Options**

- -z compresses using gzip program
- **-c** creates an archive
- -x extracts from an archive
- displays archive content (but does not extract it)
- -v displays information on the terminal window
- **-f** uses specified file
- set the current dates to extracted files

type of action

# Archiving and extracting data

Highly recommended filename extensions:

- .tar for all archives
- .gz for gzip compressed archives

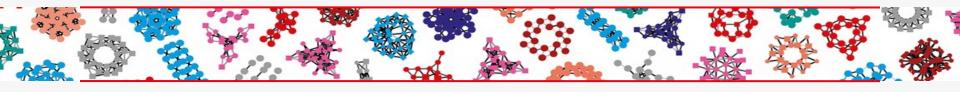
Tip: -f option must be placed at the last position because it requires argument (file name)

## In a nutshell

- Directory and file manipulation
  - mkdir, mv, cp, rm, rmdir
- Finding files and directories (find)
  - Wildcards characters for file search and display
- File determination (file)

Archiving/extracting files (tar)

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# Working with file content







# Line by line

Rule:

Content search is performed line by line

## File content statistics

#### WC

wc option filename(s)

#### **Options**

- -I prints the number of lines
- -w prints the number of words
- -c prints the number of bytes
- -m prints the number of characters

Without options, **wc** outputs the number of lines, words and bytes

# File content display: head & tail

#### head

aims at quickly showing the beginning of a file

```
head myfile.txt -> displays the first 10 lines (default)
head -2 myfile.txt -> displays the first 2 lines
head -n-2 myfile.txt -> displays all the lines, except the last 2
```

#### tail

• is similar to **head**, but shows the **last lines** of a file

```
tail myfile.txt -> displays the last 10 lines

tail -2 myfile.txt -> displays the last 2 lines

tail -n+2 myfile.txt -> displays all lines except the first (useful e.g. to remove header line)
```

# File content display: cat & less

cat displays the content of a text file

When several files are passed as arguments, cat concatenates and displays their content, thus can be used to merge the content of several files

# File content display: cat & less

#### less

displays the content of a text file one screen at a time

#### **Option**

-N shows line numbers at the left of each line

#### Useful commands to be used inside the text file:

- [space-bar], shows the next page, one screen at a time
- up/down arrow keys, moves the content backward/forward one line at a time
- < and > to reach the beginning and the end of the document
- /mouse: search the string "mouse"
- **q** to quit

### Text editors

Interactive use -> no need for text edition

Programmning -> need for text edition

Several programs available: Sublime Text, Visual Studio Code, etc

Vim is a text editor integrated into most terminals

Nano

#### UNIX has three standard streams

- Standard input stdin, where programs receive data from:
  - from the keyboard
  - from a file (using <)</li>
- **Standard output stdout**, where programs write their output data to:
  - **printed** on the terminal window
  - written in a file (using > or >>)

- Standard error stderr, to output error messages
  - **printed** on the terminal window

Example of **standard input** from file

< not mandatory with most programs

Example of standard output to a file

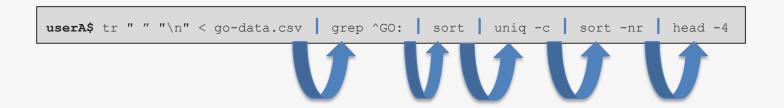
#### Command > filename

- if the file does not exist, it is created
- If it does, its content is overwritten

#### Command >> filename

- if the file does not exist, it is created (same function as >).
- If it does, the output is **added at the end** of the file content.

Output redirection: the | (pipe):



useful to pass directly the output from one program as the input of another without creating intermediate files

# Delimiter-Separated Values (DSV)

#### Free-text (not DSV)

Hello, I will be very busy the next couple of months: I started a course in Bioinformatics!

#### Comma/Semicolon-separated values (CSV)

```
Entry, Entry_name, Protein_names
Q8QMT5, A18_CWPXB, Transcript termination protein A18
Q80DV6, A18_CWPXG, Transcript termination protein A18
```

#### **Tab-separated values (TSV)**

```
Entry Entry name Protein name

Q8QMT5 A18_CWPXB Transcript termination protein

A18 Q80DV6 A18_CWPXG Transcript termination

protein A18
```

text identification, retrieval and manipulation is more efficient when structured with delimiters

# Delimiter-Separated Values (DSV)

Biological sequences are often represented in a so-called **FASTA** format:

- a first line starting with '>' and free text / comments (header line)
- main lines composed of one-letter code sequences

>sp|Q1PE49|40N1\_ARATH Protein At-4/1 OS=Arabidopsis thaliana MAATSDEQMNLLLSSFDQIYEDFKIGLNEINVYRSKSNVESSRREVLEISNKNLKEENER LKKLYTESLNNFADQLEHRTKCHSLKEELKRVNDENKSKEHEHRNALESLRQKHVTKVEE

## Newline character

structured formats → a 'newline' character\* at the end of each line, which IS NOT the same for all OS

- \n -> Unix, Mac OS X
- \r -> Mac OS (before X)
- \r\n -> Windows OS

\*use command *od -c* to view them

conversion is sometimes necessary

# Converting file content

To convert newline characters...

tr (for 'translate') can do this in a single command line:

tr '\r' '\n' < myfile > mynewfile

**tr** is very convenient to change a delimiter, e.g. from TSV to CSV

If you want to replace words or phrases, the command **sed** is required (not discussed during this course)

# Sorting file content

#### sort

- used to sort lines of text files
- default is alphabetical order

### **Options**

- -n for a numeric sort
- **-r** for reverse sort
- -u for unique lines (keeps one instance when identical lines)
- -k sorts via a key (a column number for example)
- -t to define a key separator (e.g. a |). Default is space, but tab is recognized too

sort -k is useful if you want to sort according to only some parts of a line, typically columns

## Searching / filtering file content

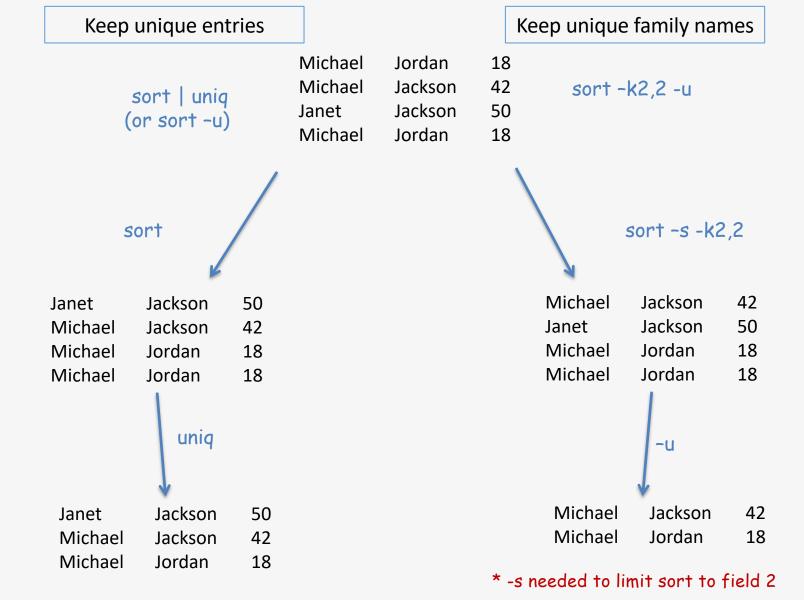
### uniq

 reports unique lines by suppressing multiple occurrences of identical lines if sequential.
 Therefore, it is typically used after sort

### **Options**

- -d, outputs only lines that are repeated (duplicated or more) in the input
- -c, precedes each reported line with the number of occurrences found
- -i, ignores the differences in case when comparing the lines
- -u, only prints unique lines

sort | uniq and sort -u have the same function: suppression of multiple occurrence of identical lines and ordering, but sort has an option (-k) to sort on specific key (e.g. a column) instead of the entire line.



## Filtering / extracting file content

**cut** is used to extract selected parts of lines (like columns). Convenient to manipulate delimiter-separated value files

### **Options**

- -c, selection based on characters positions. This is used when cut has to be performed at a fixed position (e.g. to remove a fixed header)
- -d, type of delimiter (default is 'tab'), e.g. ';' ',' ' or any character
- -f, selection based on fields in DSV files.
   single field number (e.g. -f 1), multiple field numbers (e.g. -f 1,4) or a range (e.g. -f 1-4) must be indicated. Fields are determined by delimiters if not TAB

NB: cut -f 1 | sort -u and sort -k1,1 -u are almost identical but the former will display only the extracted column

# Comparing file content

diff compares 2 files and outputs the differences.

Useful to compare:

- 2 files with the same name in different directories
- different versions of the same file

### **Options**

- -b, ignores differences in amount of white space
- -B, ignore differences of blank lines
- -s, reports when two files are identical (it does not by default)
- -q, reports only whether two files differ, no details of the differences

## Merging file content

#### cat

- display function -> can be used to concatenate content from several files
- concatenation does not include any blank or newline

#### **Options**

- -s , squeezes multiple adjacent empty output lines
- -b, numbers nonempty output lines

### paste

can merge columns from different files

#### **Options**

-d allows to introduce delimiters between columns (':' ',' '-')

## Searching file content

### grep

 for Global Regular Expression Print - searches file(s) for words or patterns and return matching lines grep [options] 'pattern' file(s)

### **Options**

- -c, displays the number of resulting lines instead of the lines themselves
- -i, performs a case insensitive search
- -v, displays lines that DO NOT match the pattern
- -o, returns only the pattern, not the entire line
- -n, adds the line number in front of the result lines
- -r, search all files recursively inside each directory

## Regular Expressions

Characters used to search a pattern, example:

<b>^</b> a	'a' at the beginning of a line
a\$	'a' at the end of a line
^\$	to express a blank line
^.\$	any character on a line
[abc]	either character
[a-z]	a lowercase character
[0-9]	any figure
[0-59]	0, 1, 2, 3, 4, 5 or 9
[^0-9]	any character except a figure

## In a nutshell

- UNIX allows to manipulate file content, such as order lines, cut fields, merge file content
- UNIX allows complex searches to retrieve filtered data
- Complex commands might be written into scripts
- Note that other languages are better suited to this sort of complex manipulations, like AWK, perl, python, or R

## Next step

UNIX shell scripting in Life Sciences
By Thomas Junier & Robin Engler
13-15 June 2023
Lausanne

https://www.sib.swiss/training/course/20230606\_ADVUN

## Further resources

### Our e-learning tutorial:

https://edu.sib.swiss/course/view.php?id=82

#### Resources that could be of interest:

http://en.wikipedia.org/wiki/List\_of\_Unix\_commands

http://www.catonmat.net/projects/cheat-sheets/

https://ubuntudanmark.dk/filer/fwunixref.pdf

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